Physical Review B - Condensed Matter and Materials Physics 2011 vol.84 N15

59Co NMR evidence for charge and orbital order in the kagome-like structure of Na 2/3CoO 2

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Abstract

We report a complete set of 59Co NMR data taken on the x=2/3 phase of sodium cobaltates Na xCoO 2 for which we have formerly established the in-plane Na ordering and its three-dimensional stacking from a combination of symmetry arguments taken from Na and Co NQR/NMR data. Here, we resolve all the parameters of the Zeeman and quadrupolar Hamiltonians for all cobalt sites in the unit cell and report the temperature dependencies of the NMR shift and spin lattice relaxation T 1 data for these sites. We confirm that three nonmagnetic Co3 + (Co1) are in axially symmetric positions and that the doped holes are delocalized on the nine complementary magnetic cobalt sites (Co2) of the atomic unit cell. The moderately complicated atomic structure resumes then in a very simple electronic structure in which the electrons delocalize on the Co2 kagome sublattice of the triangular lattice of Co sites. The observation of a single temperature dependence of the spin susceptibilities indicates that a single band picture applies, and that the magnetic properties are dominated by the static and dynamic electronic properties at the Co2 sites. We evidence that they display a strong in-plane electronic anisotropy initially unexpected but which agrees perfectly with an orbital ordering along the kagome sublattice organization. These detailed data should now permit realistic calculations of the electronic properties of this compound in order to determine the incidence of electronic correlations. © 2011 American Physical Society.

http://dx.doi.org/10.1103/PhysRevB.84.155112